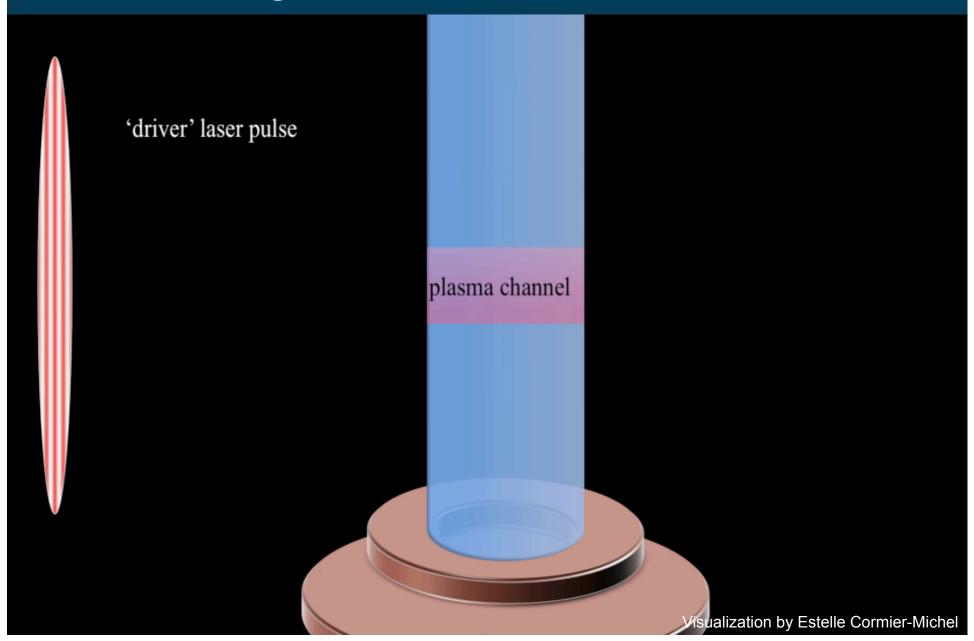
## Computational accelerator science needs towards laser-plasma accelerators for future colliders

C. G. R. Geddes, J.-L. Vay, C.B. Schroeder,

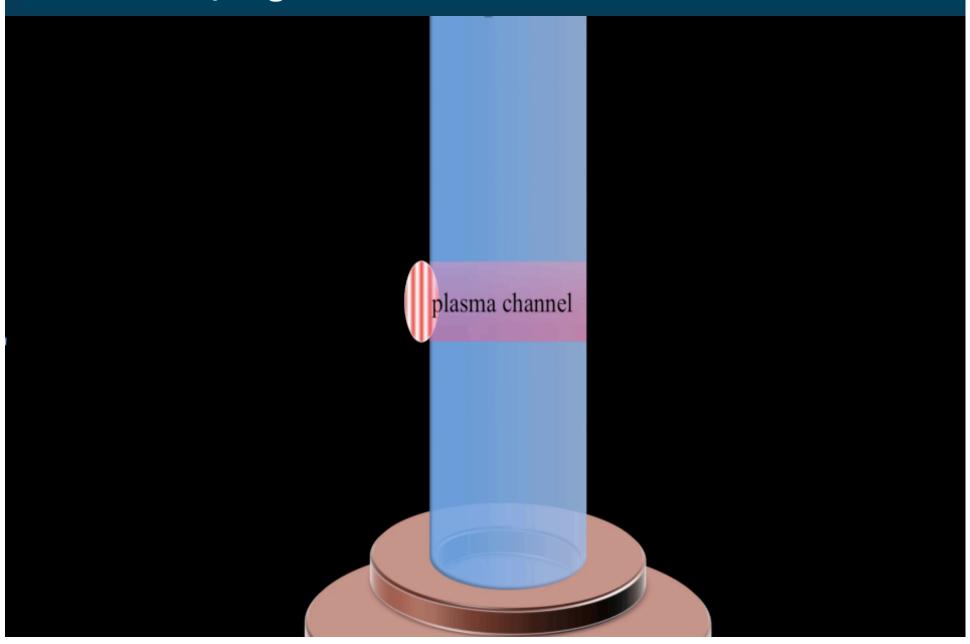
E. Esarey. W.P. Leemans

**Lawrence Berkeley National Laboratory** 

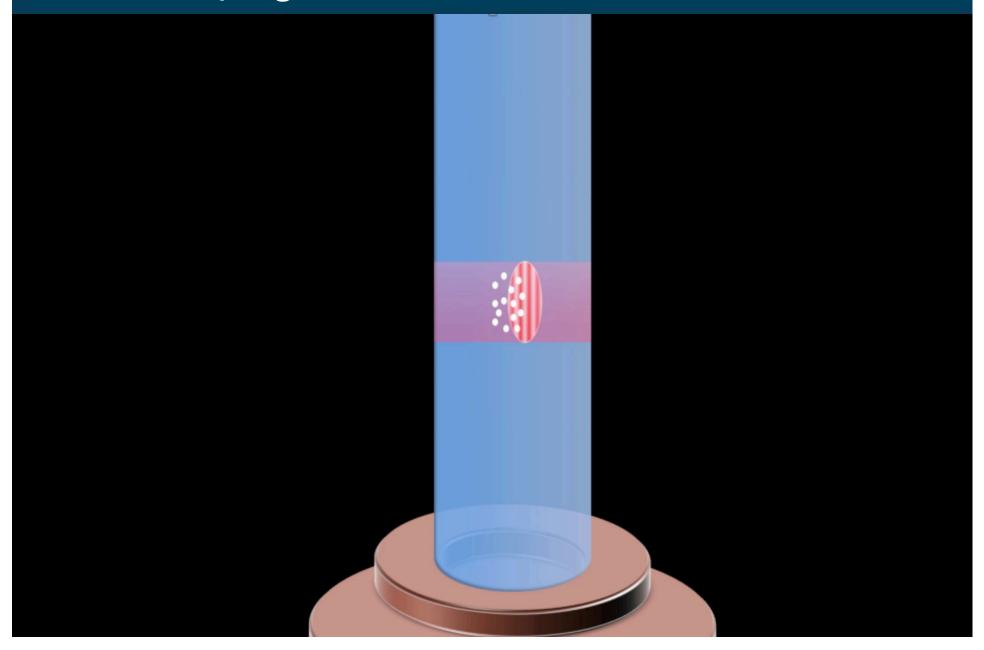
#### Laser Plasma Accelerators : ≥ 10 GeV/m gradient to reduce size of future linacs



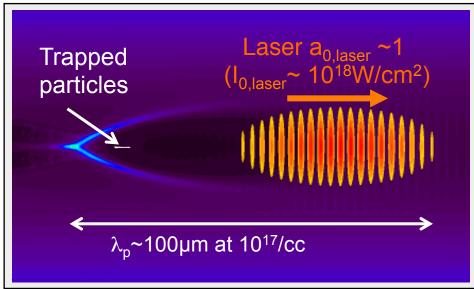
#### Laser Plasma Accelerators : ≥ 10 GeV/m gradient to reduce size of future linacs



#### Laser Plasma Accelerators : ≥ 10 GeV/m gradient to reduce size of future linacs



## Laser Plasma Accelerators\*: ≥ 10 GeV/m gradient to reduce size of future linacs



Space charge restoring force -> wakefield

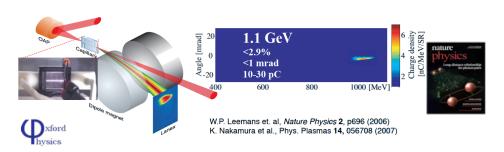
$$T_{laser} < T_{plasma} \sim 50 fs$$

Accelerating fields ~ GeV per cm

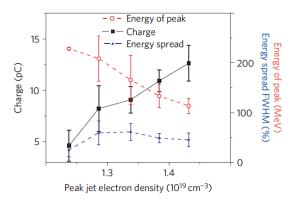
Wake velocity ~ laser velocity



## Laser Plasma Accelerators produce GeV beams with low emittance and ΔE

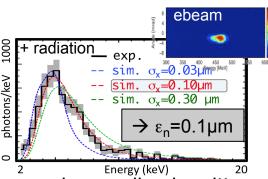


GeV beams in 3 cm capillary
→PW lasers such as BELLA¹ producing 2 GeV, targeting 10 GeV
Leemans et al, Nature Physics 2006



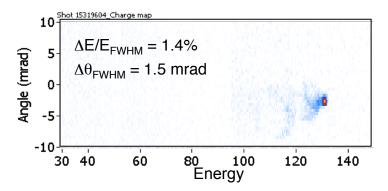
#### Controlled injection & performance

Gonsalves et al., Nature Physics 2011 Related: Faure Nature Physics 2006



0.1 mm-mrad normalized emittance

Plateau et al, PRL 108, 2012 Related: Weingartner PRL 2012



1% level integrated energy spread sub – 1% slice energy spread

Related: Lin et al, PRL 108, 2012

Experiments on staging of multiple modules to increase energy are in progress<sup>2</sup>

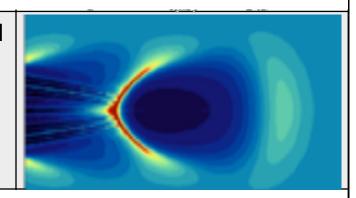
# LPA Simulation: EM plasma, with gas dynamics, radiation/scattering

Time	Physics	Codes	Example
scale			

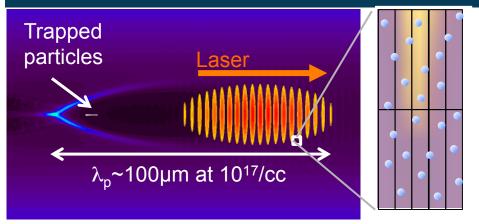
Laser-plasma interaction, focusing, ionization, depletion.
Injection/evolution of particle beams

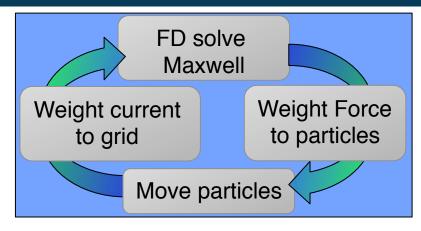
EM Fluid, Particle-In-Cell

VORPAL, INF&RNO, ALaDyn, WARP, REMP Related: OSIRIS, QuickPIC, VLPL...



# Core simulation: EM plasma scales well, models cm-scale GeV LPAs





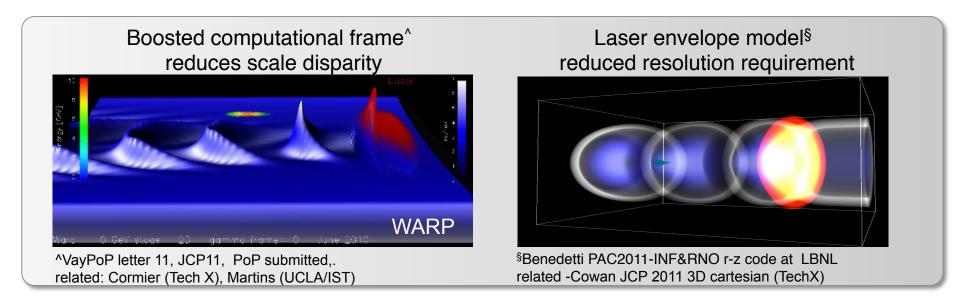
#### **Explicit PIC/fluid simulates core LPA physics**

- Scale to >100kcore via domain decomposition
- Limits include area/volume and I/O scaling

#### For future high energy and high quality beams:

- Laser-to-plasma scale separation limits m-scale and beyond
- Accuracy issues: noise, numerical temperature, staggered grid

## Plasma-physics based reduced models allow 10 GeV meter-scale simulations



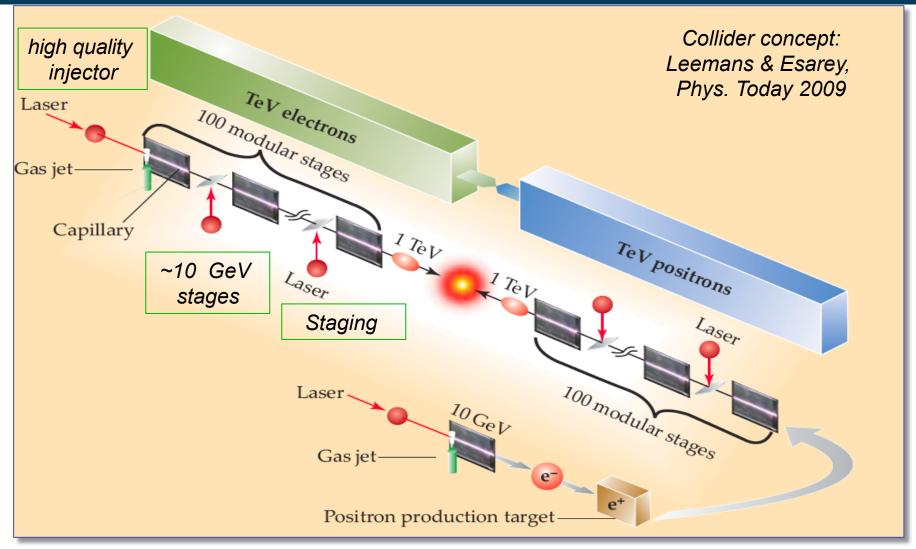
#### Supported design of BELLA PW laser and collider concepts<sup>1</sup>

Full scale required for correct emittance, focusing

#### Coupled with methods to reduce unphysical kinetic effects

High order particles, smoothing, controlled dispersion and push

## Research focus: Physics/R&D challenges towards detailed conceptual design of a future collider



- Intermediate applications include FEL and Thomson gamma light sources
- Research needs detailed in Facilities group paper by J.P. Delahaye et al.

## Physics capabilities for high-energy physics LPAs

Staging: order 100 LPAs, each of meter scale

Resolution of 10 nm – scale emittance

- Compact beam cooling methods
- Including scattering and radiation effects

Spin polarization and preservation

Positron production and acceleration/focusing

Compact final focus methods (e.g. adiabatic plasma lens)

# LPA Simulation: EM plasma, with gas dynamics, radiation/scattering

Time scale	Physics	Codes	Example	
ms	Gas target formation: capillaries and gas jets	Gas dynamics- ANSYS, OpenFOAM		
ns	Plasma formation in capillary discharges	MHD - Bobrova	0.004 n(le24/cc) 5.2	
ps/fs	<ul> <li>Laser-plasma interaction, focusing, ionization, depletion.</li> <li>Injection/evolution of particle beams</li> </ul>	VORPAL, INF&RNO, ALaDyn, WARP, REMP Related: OSIRIS, QuickPIC, VLPL		
	FEL, radiation, beam transport	GINGER, VDSR, GPT	200000 150000 100000 50000 0 0 80 160 240 320 400	

#### Radiation and Scattering models

#### Radiation from oscillations in strong focusing fields

Used for betatron, Thomson scattering

#### Scattering from plasma particles, foils

#### **Presently external to LPA simulations**

For collider distances / emittances integration to LPA sim. required

## Computing capabilities for high-energy physics LPAs

#### Length of simulation and emittance accuracy increase 1-2 orders

■ Domain size similar → weak scaling limited

#### Integrate models for e+ production, radiation, polarization

- Resolve quantization of radiation
- Correct statistics require increased particle number

Computing methods/requirements detail: http://www.nersc.gov/science/hpc-requirements-reviews/HEP/case-studies/

# Common to many codes

## Accelerator modeling science capabilities for high-energy physics LPAs

#### Scaling for particle number and resolution. Require:

- Common I/O libraries that achieve full bandwidth
- Parallel analysis with advanced mathematics, in-sit

#### Multicore/SIMD work well with PIC

Need common tools, test beds, advance notice, het. decomp.

#### Compute power increasing faster than bandwidth

High accuracy/long timestep methods, even at higher cost

#### New models for improved accuracy/ momentum fidelity

- Spectral, nodal, integrate accel. codes...
- Vlasov

## Supporting capabilities for high-energy physics LPAs

#### **Target formation**

- 3D plasma formation including flow
- Heat deposition from laser
- Heat flow and extraction at kHz- MHz

#### Beam transport of fs, multi-kA beams

#### High average power lasers

Materials, optical propagation/amplification, heat flow

## Compute needs driven by requirement for Accuracy, low emittance, and 100-stage sim.

#### Estimates based on physics needs

	Present	5 years	10 years
Computation (Mhours)	15	500	10,000
Typical cores* for production runs	5000	50,000	50,000
Maximum cores* for production	16000	250-500k	5M
Data read and written per run (TB)	3 TB	100 TB	1000 TB
Minimum I/O bandwidth	0.3 GB/sec	10 GB/sec	100 GB/sec
Shared file-system space	20 TB	600 TB	6 PB
Memory requirement per core.	0.1 GB	0.1 GB	0.2 GB

#### **Summary**

EM PIC/fluid supported exp. at GeV in few cm,  $\Delta E^{1}$ ,  $\epsilon_{n}^{0.1}$  um

#### Address challenges for detailed conceptual design of a future collider

- 100's of 10 GeV stages, 0.01 um level  $\varepsilon_n \rightarrow$  length, accuracy
- Integrate: e<sup>+</sup>, radiation, scattering, polarization...
- Add: Cooling, focusing, 3d target formation, heat flow, laser

#### **Requires combination of:**

 Scaling (incl. I/O & analytics), new physics models/solvers, new computing architectures

## White paper on DOE-HEP Accelerator Modeling Science Activities

J.-L. Vay, <u>C. G. R. Geddes</u>
Lawrence Berkeley National Laboratory

A. Friedman, D. P. Grote Lawrence Livermore National Laboratory

D. L. Bruhwiler
University of Colorado

#### Goal (from the draft charge):

"maximizing the impact of computer modeling on the design of future particle accelerators and the development of new accelerator techniques & technologies."

#### This white paper presents the rationale for:

- a. strengthening and expanding programmatic activities in accelerator modeling science within DOE-HEP,
- b. increasing the community-wide coordination and integration of code development.

#### Importance of modeling is on the rise

#### with increasing:

- pressure for reducing uncertainties and cost on development, construction & commissioning of accelerator,
- accuracy of codes with better algorithms and more physics,
- computers capacity.

#### Resources optimization calls for balanced approach

#### Maximizing the overall scientific output/\$ means:

- maximizing usability of the pool of codes:
  - effectiveness (completeness, accuracy of solution),
  - efficiency (time to solution),
  - ease of use (learnability, error tolerance, versatility, etc.),
- while minimizing spending on development and support:
  - reduction of duplication,
  - increase in modularity and code interoperability.

#### Implies comprehensive strategy that evaluates codes

- not only based on performance, effectiveness, ease of use, levels of documentation and support,
- but also on other attributes such as modularity, flexibility, reusability, expandability and interoperability.

#### March toward exascale brings extra challenges

#### **Next generation of High Performance Computers**

- will provide high-accuracy integrated simulations, better design optimization, near real-time modeling, ...
- eventually leading to virtual accelerators (including virtual "control room").

#### But with increased heterogeneity and level of parallelism:

→ programming of next generation computers will require **new** or **reworked codes** with **new exascale-ready algorithms**.

#### **Beam & Accelerator Modeling Science**

#### is increasingly relevant as a programmatic activity:

- timely to go beyond code development and application in support of theory and experiments,
- development and application of accelerator algorithms/codes are very complex and specialized tasks,
- need for dedicated teams within HEP (in collab. w/ ASCR):
  - physicists + applied math + computer scientists
  - to develop codes w/ more physics on more complex machines
  - examples elsewhere of such dedicated teams:
    - MPI Garching, Germany MFE-ITER
    - Saclay, France CILEX-LPA/laser applications

#### Need for coordination into a cohesive tool set

#### Numerous beam/accelerator codes developed worldwide:

- offer wide array of options to modelers,
- but cohesion is lacking, w/ some duplication & inefficiency.

#### Usual paradigm (with very few exceptions):

- one developer (physicist)/topic/project
  - occasional help from computer scientist/applied math.
- leads to many small specialized codes
  - lack breadth required for integrated multi-physics modeling

#### Integrated multi-physics modeling calls for more cohesion

#### Portfolio should cover from low- to high-end computing

#### Supercomputers aggregate of many "off-the-shelf" units:

- each unit similar or same as on desktops or laptops
- development now often on laptops/desktops/small clusters:
  - faster turnaround for development, testing, debugging

#### Desktops/laptops are becoming more powerful

- will soon integrate tens of cores
- can tackle many low- to medium- range modeling

Separation between low- & high-end computing is vanishing

Need comprehensive program covering low- to high-end

#### Need and solution for non-disruptive integration

#### Significant investments of HEP into existing pool of codes:

- essential to minimize disruptions to developers and users,
- while enabling interoperability and expandability.

#### Python scripting language has unique attributes:

- rapid development and prototyping of scientific applications
  - on par with e.g. Maple, Matlab (which it is often supplanting)
- is expandable and couples to FORTRAN, C and C++

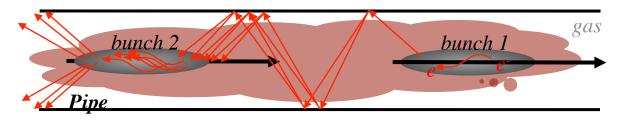
#### Ideal for coupling existing codes with minimized disruptions

- codes continue unmodified but functionalities are exposed
- → integrated tool set of unprecedented power and versatility.

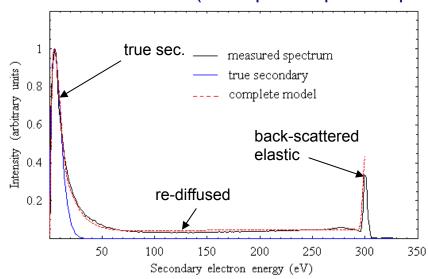
## Example #1: Warp and Posinst integrated in a modular "combo" package

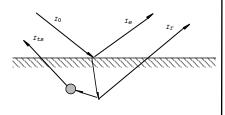
#### Enabling fully self-consistent modeling of e-cloud effects: build-up & beam dynamics:

 Beyond standard practice of simulating e- cloud buildup (ECLOUD, Vorpal, etc) and then its effect on beams (Headtail, SYNERGIA, etc)



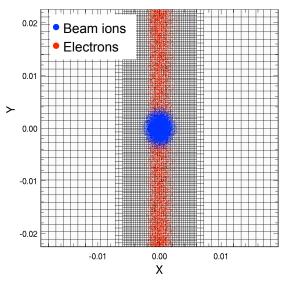
#### Posinst provides advanced secondary electrons model (and optional particle pusher).





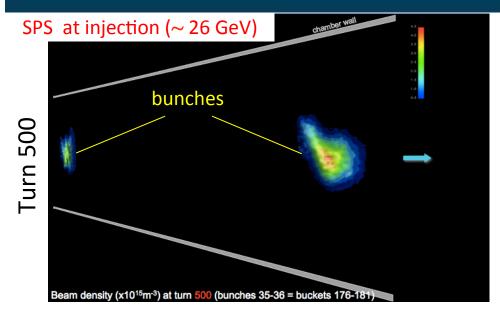
Monte-Carlo generation of electrons with energy and angular dependence.

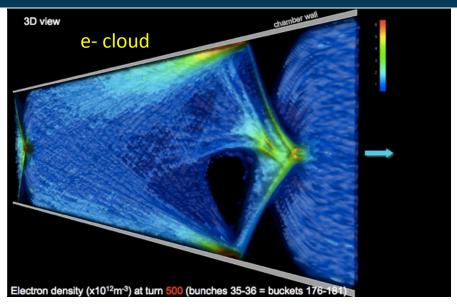
#### Warp's mesh refinement & parallelism provide efficiency.



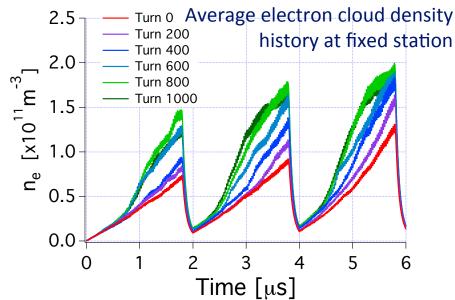
Python programming language is the glue between Warp and Posinst

### First direct simulation of a train of 3x72 bunches -- using 9,600 CPUs on NERSC supercomputer





• Unexpected e<sup>-</sup> density rise in tails of batches between turns 0 and 800\*.



## Example #2: Warp & Icool combined with Python and applied to muon cooling in US MAP

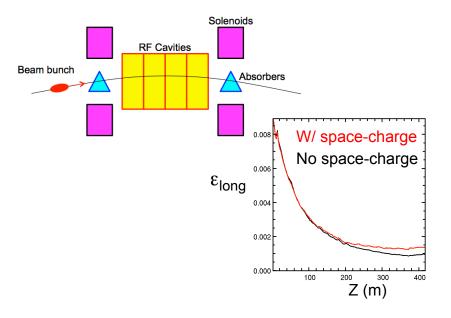
Warp: particle tracking plus self fields

**ICOOL**: absorption

#### No changes to ICOOL (except skipping main routine)

Particle handling in Python – passing appropriate particles to ICOOL

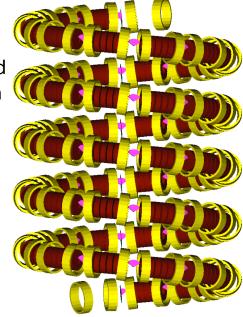
Initial 2-D RZ simulation results show reduced cooling when including space-charge



Full characterization requires 3-D (in progress):

Current cooling lattice is a tapered helical line

 Simulation needs to include curvature and transverse dispersion



#### **Summary**

#### (a) Expanding accelerator modeling science activities

- importance of modeling is on the rise
  - better codes, computers, pressure to control cost
- resources optimization calls for balanced approach
  - emphasize also modularity, interoperability, ...
- march toward exascale brings extra challenges
  - requires new codes with new exascale-ready algorithms
- needs programmatic beam/accelerator modeling science
  - with integrated teams (phys. + math. + comput.)

#### **Summary**

#### (b) Increasing community-wide coordination & integration

- need for coordination into a cohesive tool set
  - integrated multiphysics modeling calls for more cohesion
- portfolio should cover from low- to high-end computing
  - separation between low- & high-end computing is vanishing
- need for non-disruptive integration
  - many existing codes used by many users for study & design
- Python stands out as solution for progressive coupling
  - codes continue unmodified but functionalities are exposed
  - → integrated tool set of unprecedented power and versatility.

#### **Backup material**

## BELLA laser in operation at LBNL: 10 GeV Collider relevant module

- State of the art 1 PW, 1Hz, 40 fs
  - Commercial system with Strehl > 0.9
- Simulations show 10 GeV in 0.1-0.5 m experiments in progress

